Towards a New ODE Solver Based on Cartan's Equivalence Method

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ABSTRACT

The aim of the present paper is to propose an algorithm for a new ODE–solver which should improve the abilities of current solvers to handle second order differential equations. The paper provides also a theoretical result revealing the relationship between the change of coordinates, that maps the generic equation to a given target equation, and the symmetry $\mathcal{D}$-groupoid of this target.

Categories and Subject Descriptors

I.1.2H.4 [**Symbolic and Algebraic Manipulation**]: Computing Methodologies—*Algorithms*

General Terms

Algorithms

Keywords

ODE-solver, differential algebra, equivalence problems, Cartan's equivalence method

1. INTRODUCTION

Current ODE-solvers make use of a combination of symmetry methods and classification methods. Classification methods are used when the ODE matches a recognizable pattern (that is, for which a solving method is already implemented), and symmetry methods are reserved for the non-classifiable cases – Fig. 1. Using symmetry methods, the solvers first look for the generators of 1-parameter symmetry groups of the given ODE, and then use this information to integrate it, or at least reduce its order [4, 5].

In practice, present solvers are often unable to return closed form solution. Consider for instance the following equation

$$y'' = -y^3 y'^4 - \frac{y'^2}{y} - \frac{1}{2} y, \qquad (1)$$

ISSAC'07, July 29–August 1, 2007, Waterloo, Ontario, Canada.

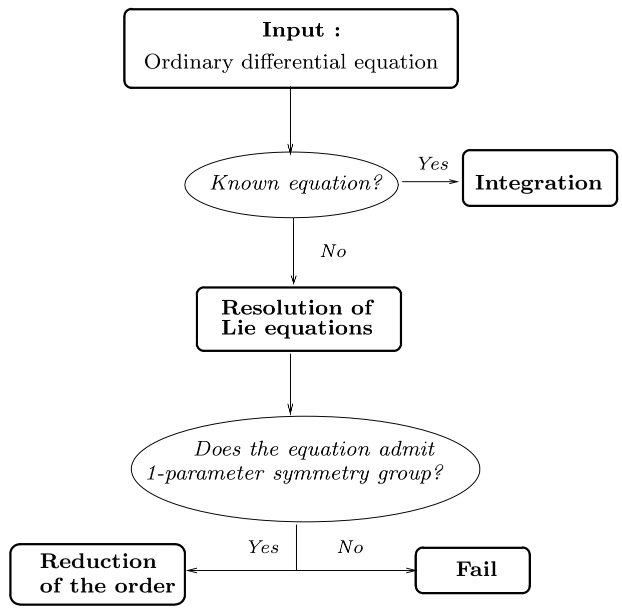

Figure 1: *General flowchart of typical ODE-solver.*

which admits only one 1-parameter symmetry group. Using this information, actual solvers return a complicated first order ODE and a quadrature. Clearly, such output is quite useless for practical applications. More dramatically, consider the following equation

$$y'' = \frac{2\,x^4 y' - 6\,y^2 x - 1}{x^5}. \qquad (2)$$

When applied actual solvers, output no result. This failure is due to the fact that the above equation does not match any recognizable pattern and has zerodimensional point symmetry group(oid). Thus neither symmetry method nor classification method works.

Our solver (the implementation is in progress) is designed to handle such equations. It returns an equation from Kamke's book [9], equivalent to the equation to be solved, and the equivalence transformation φ. Thus, for the equation (1) we obtain the Rayleigh equation $y'' + y'^4 + y = 0$ (number 72 in [9]) and the change of coordinates $\varphi : (x, y) \to (x,\, y^2/2)$. For the equation (2), we obtain the first Painlevé equation $y'' = 6y^2 + x$ (number 3 in [9]) and the change of coordinates $\varphi : (x, y) \to (1/x,\, y)$. It is worth noticing that this transfor-

mation can be composed with the point symmetries of the Painlevé equation given by $(x, y) \to (\lambda^2 x,\ \lambda y)$ with $\lambda^5 = 1$.

To summarize the theoretical result of the paper, let $\mathcal{E}_f$ denote the generic ODE $y'' = f(x, y, y')$ and Φ an allowed $\mathcal{D}$-groupoid acting on the variables x and y. Suppose that Φ is given by quasi-linear Lie defining equations. Define $\mathcal{S}_f := \mathrm{aut}(\mathcal{E}_f) \cap \Phi$ where $\mathrm{aut}(\mathcal{E}_f)$ denotes the (local) contact symmetry $\mathcal{D}$-groupoid of $\mathcal{E}_f$. Given $\bar{f} \in \mathbb{Q}(x, y, y')$ and assume that the symmetry $\mathcal{D}$-groupoid $\mathcal{S}_{\bar{f}}$ is zerodimensional. The transformation $\varphi \in \Phi$ mapping the generic equation $\mathcal{E}_f$ to the target equation $\mathcal{E}_{\bar{f}}$ is called the *necessary form of the change of coordinates*. We shall see that this transformation exists and belongs to the differential field $\overline{\mathbb{Q}\langle f \rangle}$, endowed with the partial derivations $(\partial_x,\ \partial_y, \partial_{y'})$, for almost any analytic function f satisfying $\varphi_*(\mathcal{E}_f) = \mathcal{E}_{\bar{f}}$. In other words, φ is an algebraic function in f and its partial derivatives and can be obtained without solving differential equations. Moreover, the degree of φ is equal to $\mathrm{card}(\mathcal{S}_{\bar{f}})$ which is finite. Note that, the use of the $\mathcal{D}$-groupoids formalism is dictated by the non global invertibility of the transformation φ.

As we shall see, φ can be obtained using differential elimination. Unfortunately, such approach is rarely effective due to expressions swell. For this reason, we propose in section 4 a new method to precompute the transformation φ in terms of differential invariants, for each target equation $\mathcal{E}_{\bar{f}}$ in Kamke's list. These invariants are provided by Cartan's method. In the last section, we present our solver. This solver uses 7 possible types of transformations $\Phi_1, \cdots, \Phi_7$. Using Lie infinitesimal method we precalculate to each target equation a signature. That is, the dimensions of the 7 symmetry groupoids associated to the 7 groupoids $\Phi_1, \cdots, \Phi_7$. If two differential equations are equivalent then their signatures *match*. This fact significantly restricts the space of research in kamke's list at the run-time (when the input equation $\mathcal{E}_f$ is known).

2. EQUIVALENCE PROBLEMS

2.1 Groupoids

Definition 1 (Groupoid). *A* groupoid *is a category in which every arrow is invertible.*

Let $(\mathcal{G}, \circ, \mathrm{s}, \mathrm{t})$ be a category. Each arrow $\varphi \in \mathcal{G}$ admits a source $\mathrm{s}(\varphi)$ and a target $\mathrm{t}(\varphi)$ which are *objects* of this category. For each arrows $\alpha,\ \beta \in \mathcal{G}$ such that $\mathrm{s}(\beta) = \mathrm{t}(\alpha)$, there exists a unique arrow $\beta \circ \alpha \in \mathcal{G}$ with the source $\mathrm{s}(\alpha)$ and the target $\mathrm{t}(\beta)$. If $\mathcal{G}$ is a groupoid, for each arrow $\varphi \in \mathcal{G}$, there exists a unique inverse arrow φ^{-1} such that $\varphi^{-1} \circ \varphi = \mathrm{Id}_{\mathrm{s}(\varphi)}$ and $\varphi \circ \varphi^{-1} = \mathrm{Id}_{\mathrm{t}(\varphi)}$.

Let X and U be two manifolds and $\mathrm{x} \in X$. The Taylor series up to order q (i.e. the jet of order q) of a function $f : X \to U$, of class C^q, is denoted $\jmath^q_{\mathrm{x}} f$. The Taylor series of f about x is denoted $\jmath_{\mathrm{x}} f$ or $\jmath^{\infty}_{\mathrm{x}} f$. We shall say that $\mathrm{x} \in X$ is the source and $f(\mathrm{x}) \in U$ is the target of the q-jet $\jmath^q_x f$.

Example 1. *For instance, when $X = U = \mathbb{C}$, we have*

$$\jmath^q_x f := \left(x, f(x), f'(x), \ldots, f^{(q)}(x)\right) \in \mathbb{C}^{q+2}.$$

This jet is said to be invertible *if $f'(x) \neq 0$. The jet of the function* Id *about the point x is $(x, x, 1, 0, \ldots, 0)$.*

For each $q \in \mathbb{N}$ and each $\mathrm{x} \in X$, we set $\mathrm{J}^q_{\mathrm{x}}(X, U) := \bigcup_f \jmath^q_{\mathrm{x}} f$ and $\mathrm{J}^q(X, U) := \bigsqcup_{\mathrm{x} \in X} \mathrm{J}^q_{\mathrm{x}}(X, U)$. We denote by $\mathrm{J}^q_*(X, X)$ the submanifold of $\mathrm{J}^q(X, X)$ formed by the invertible jets. $\mathrm{J}^q_*(X, X)$ is a groupoid [14] for the composition of Taylor series up to order q according to

$$\jmath^q_{\mathrm{x}}(g \circ f) = \left(\jmath^q_{f(\mathrm{x})} g\right) \circ (\jmath^q_{\mathrm{x}} f)\,. \tag{3}$$

By definition, a $\mathcal{D}$-groupoid [12] $\mathcal{G} \subset \mathrm{J}^{\infty}_*(X, X)$ is a sub–groupoid of $\mathrm{J}^{\infty}_*(X, X)$ formed by the Taylor series solutions (see def. 8) of an algebraic PDE system called the *Lie defining equations*. This system contains an inequation which expresses the invertibility of the jets. The set of smooth functions $\varphi : X \to X$ that are local solutions of the Lie defining equations of $\mathcal{G}$ is a *pseudo-group* denoted by $\Gamma\mathcal{G}$. We define $\dim \mathcal{G} := \dim C$ and, if $\dim C = 0$, $\deg \mathcal{G} := \deg C$ where C is a characteristic set (see sect. 3) of the Lie defining equations. We have $\deg \mathcal{G} = \mathrm{card}(\Gamma\mathcal{G})$.

Example 2 (Φ_3). *Let Φ_3 (see table 1) be the $\mathcal{D}$-groupoid of infinite jets of transformations $(\bar{x}, \bar{y}) = \varphi(x, y)$ where*

$$\bar{x} = x + C \text{ and } \bar{y} = \eta(x, y). \tag{4}$$

The constant $C \in \mathbb{C}$ and the function $\eta : \mathbb{C}^2 \to \mathbb{C}$ are arbitrary. $\Phi_3 \subset \mathrm{J}^{\infty}_*(\mathbb{C}^2, \mathbb{C}^2)$ is an infinite dimensional $\mathcal{D}$-groupoid where the corresponding Lie defining equations are

$$\bar{x}_x = 1,\ \bar{x}_y = 0,\ \bar{y}_y \neq 0. \tag{5}$$

Definition 2 ($\mathcal{G}$-Invariant). *An* invariant *of the $\mathcal{D}$-groupoid $\mathcal{G} \subset \mathrm{J}^{\infty}_*(X, X)$ is a function $I : X \to \mathbb{C}$ which is constant on the orbits of $\mathcal{G}$.*

Clearly, the sum, the product and the ratio of two invariant functions is still an invariant function. Consequently, invariant functions of $\mathcal{G}$ define a field.

2.2 Differential equations and diffieties

Let $\mathcal{E}_f$ denotes the generic ODE

$$y^{(n+1)} = f(x,\, y,\, y', \ldots,\, y^{(n)}). \tag{6}$$

Let $M := \mathrm{J}^n(\mathbb{C}, \mathbb{C})$ be the n–th order jets space [16] of functions from $\mathbb{C}$ to $\mathbb{C}$. Let $\mathrm{x} := (x,\, y,\, y_1,\, \ldots,\, y_n) \in \mathbb{C}^m$ be a local coordinates system over M where $m := n+2 = \dim M$.

Every differential equation $\mathcal{E}_f$ defines a *diffiety* [11]. This diffiety is given by the manifold M and a set of 1-forms, called *contact forms*, satisfying the Frobenius condition of complete integrability. Contact forms are linear combinations of the basic contact 1-forms $\mathrm{d}y - y_1 \mathrm{d}x$, $\mathrm{d}y_1 - y_2 \mathrm{d}x, \cdots$, $\mathrm{d}y_n - f(\mathrm{x})\mathrm{d}x$. Vector fields which are orthogonal to the contact forms are colinear to the *Cartan field*

$$D_x := \frac{\partial}{\partial x} + y_1 \frac{\partial}{\partial y} + y_2 \frac{\partial}{\partial y_1} + \cdots + f(\mathrm{x}) \frac{\partial}{\partial y_n}.$$

They generate a distribution denoted by Δ_f. A *local isomorphism* φ between two diffieties $\mathcal{E}_f$ and $\mathcal{E}_{\bar{f}}$ is, by definition, a local diffeomorphism $\varphi : M \to M$ such that

$$\Delta_{\bar{f}} = \varphi_*(\Delta_f).$$

2.3 Equivalence problem and symmetries

Definition 3 (Equivalence problem). *An* equivalence problem (EPB) *is an ordered pair (M, Φ) where $M = \mathrm{J}^n(\mathbb{C}, \mathbb{C})$ and $\Phi \subset \mathrm{J}^{\infty}_*(\mathbb{C}^2,\, \mathbb{C}^2)$ is a $\mathcal{D}$-groupoid of point transformations from $\mathbb{C}^2$ to $\mathbb{C}^2$.*

There exists a unique prolongation of Φ, denoted $\Phi^{(n)}$, that acts on M (see section 3.4.1). Two differential equations $\mathcal{E}_f$ and $\mathcal{E}_{\bar{f}}$ are said to be equivalent if there exists a local transformation $\varphi : M \to M$ satisfying the differential system

$$\Delta_{\bar{f}} = \varphi_*(\Delta_f) \text{ and } \varphi \in \Gamma\Phi^{(n)}. \qquad (7)$$

The second condition means that φ fulfills the Lie defining equations of the $\mathcal{D}$-groupoid $\Phi^{(n)}$.

The system (7) is fundamental and we shall see that it can be treated by two different approaches : brute-force method based on differential algebra (section 3) and geometric approach relying on Cartan's theory of exterior differential systems (section 4). It is classically known that the existence of at least one transformation φ can be checked by computing the *integrability conditions* of the system (7), which is completely algorithmic whenever f and $\bar{f}$ are explicitly known [3, 16, 1]. However, there is no general algorithm for computing closed form of φ. In the sequel, we shall show that if the function $\bar{f}$ is fixed such that a certain $\mathcal{D}$-groupoid $\mathcal{S}_{\bar{f}}$ is zerodimensional, then φ is obtained *without* integrating any differential equation.

Definition 4 ($\mathcal{S}_{\bar{f}}$). *To any EPB, with fixed target equation $\mathcal{E}_{\bar{f}}$, we associate the $\mathcal{D}$-groupoid $\mathcal{S}_{\bar{f}} \subset \mathrm{J}^\infty_*(M, M)$ formed by the Taylor series solutions of the* self–equivalence *problem*

$$\Delta_{\bar{f}} = \sigma_*(\Delta_{\bar{f}}) \text{ and } \sigma \in \Gamma\Phi^{(n)}. \qquad (8)$$

Example 3. *Consider the EPB $(\mathrm{J}^1(\mathbb{C},\mathbb{C}), \Phi_3)$ and the Emden-Fowler equation $\mathcal{E}_{\bar{f}}$ (number 11 in [9])*

$$y'' = \frac{1}{xy^2}. \qquad (9)$$

The Lie defining equations of the $\mathcal{D}$-groupoid $\mathcal{S}_{\bar{f}}$ are given by the characteristic set

$$\left\{\bar{p} = \frac{\bar{y}p}{y},\ \bar{y}^3 = y^3,\ \bar{x} = x\right\}. \qquad (10)$$

This PDE system is particular. Indeed, it contains only non differential equations. We have $\dim \mathcal{S}_{\bar{f}} = 0$ and $\deg \mathcal{S}_{\bar{f}} = 3$. We deduce that its associated pseudo-group

$$\Gamma\mathcal{S}_{\bar{f}} = \left\{(x, y, p) \to (x, \lambda y, \lambda p) \mid \lambda^3 = 1\right\}$$

is, actually, a group with 3 elements.

Equivalence problem and associated $\mathcal{D}$-groupoid

Let $X := \mathrm{J}^\infty(M, \mathbb{C})$. Any EPB (M, Φ) defines a $\mathcal{D}$-groupoid $\mathcal{G} \subset \mathrm{J}^\infty_*(X, X)$ formed by the set of triplets

$$(\jmath_{\mathrm{x}} f,\ \jmath_{\mathrm{x}} \varphi,\ \jmath_{\varphi(\mathrm{x})} \bar{f})$$

where $\mathrm{x} \in M$ and the functions $(f, \varphi, \bar{f})$ are local solutions of the differential system (7). The source of a triplet is the infinite jet $\jmath_{\mathrm{x}} f \in X$ and the target is the infinite jet $\jmath_{\varphi(\mathrm{x})} \bar{f} \in X$. The composition of two triplets $(\jmath_{\mathrm{x}} f,\ \jmath_{\mathrm{x}} \varphi_1,\ \jmath_{\mathrm{x}_1} f_1)$ and $(\jmath_{\mathrm{x}_1} f_1,\ \jmath_{\mathrm{x}_1} \varphi_2,\ \jmath_{\mathrm{x}_2} f_2)$ is the triplet $(\jmath_{\mathrm{x}} f,\ \jmath_{\mathrm{x}} \varphi,\ \jmath_{\mathrm{x}_2} f_2)$ where we have $\varphi := \varphi_2 \circ \varphi_1$.

Definition 5 (Specialized invariant). *For each $\mathcal{G}$-invariant I and each function $f : M \to \mathbb{C}$, we define the* specialized invariant $I[f] : M \to \mathbb{C}$ *by*

$$I[f](\mathrm{x}) := I(\jmath_{\mathrm{x}} f), \quad \mathrm{x} \in M. \qquad (11)$$

3. USING DIFFERENTIAL ALGEBRA

The aim of this section is to use differential elimination to solve the EPB when the target function $\bar{f}$ is a $\mathbb{Q}$-rational function, explicitly known and the $\mathcal{D}$-groupoid of symmetries $\mathcal{S}_{\bar{f}}$ is zerodimensional.

3.1 The vocabulary

The reader is assumed to be familiar with the basic notions and notations of differential algebra. Reference books are [18] and [10]. We also refer to [2, 8, 1]. Let $U = \{u_1, \cdots, u_n\}$ be a set of differential indeterminates. k is a differential field of characteristic zero endowed with the set of derivations $\Delta = \{\partial_1, \cdots, \partial_p\}$. The monoid of derivations

$$\Theta := \left\{\partial_1^{\alpha_1} \partial_2^{\alpha_2} \cdots \partial_p^{\alpha_p} \mid \alpha_1, \ldots, \alpha_p \in \mathbb{N}\right\} \qquad (12)$$

acts freely on the alphabet U and defines a new (infinite) alphabet ΘU. The differential ring of the polynomials built over ΘU with coefficients in k is denoted $R = \mathrm{k}\{U\}$. Fix an admissible ranking over ΘU. For $f \in R$, $\mathrm{ld}(f) \in \Theta U$ denotes the *leader* (main variable), $I_f \in R$ denotes the *initial* of f and $S_f \in R$ denotes the separant of f. Recall that $S_f = \frac{\partial f}{\partial v}$ where $v = \mathrm{ld}(f)$. Let $C \subset R$ be a finite set of differential polynomials. Denote by $[C]$ the differential ideal generated by C and by $\sqrt{[C]}$ the radical of $[C]$. Let $H_C := \{I_f \mid f \in C\} \cup \{S_f \mid f \in C\}$. As usual, full_rem is the Ritt full reduction algorithm [10]. If $r =$ full_rem (f, C) then $\exists h \in H_C^\infty$, $hf = r \mod [C]$. Then the *normal form* is defined by normal_form$(f) := r/h$.

Definition 6 (Characteristic set). *The set $C \subset R$ is said to be a* characteristic set *of the differential ideal $\mathfrak{c} := \sqrt{[C]} : H_C^\infty$ if*

(1) C is autoreduced,

(2) $f \in \mathfrak{c}$ if and only if full_rem $(f, C) = 0$.

Definition 7 (Quasi–linear characteristic set). *The characteristic set $C \subset R$ is said to be* quasi–linear *if for each $f \in C$ we have $\deg(f, v) = 1$ where v is the leader of f.*

Proposition 1. *When the characteristic set C is quasi–linear, the differential ideal $\mathfrak{c} := \sqrt{[C]} : H_C^\infty \subset R$ is prime.*

3.2 Taylor series solutions space

Let $\mathrm{k} := \mathbb{Q}(x_1, \cdots, x_p)$ be the differential field of coefficients endowed with the set of derivations $\left\{\frac{\partial}{\partial x_1}, \cdots, \frac{\partial}{\partial x_p}\right\}$. Let C be a characteristic set of a prime differential ideal $\mathfrak{c} \subset R$. We associate to C the system

$$(C = 0, H_C \neq 0) \qquad (13)$$

of equations $f = 0$, $f \in C$ and inequations $h \neq 0$, $h \in H_C$.

Definition 8 (Taylor series solution). *A* Taylor series solution *of the PDE system (13) above is a morphism $\mu : R \to \mathbb{C}$ of (non differential) $\mathbb{Q}$-algebras such that*

$$[C] \subset \ker\mu \text{ and } H_C \cap \ker\mu = \emptyset.$$

The morphism μ defines an infinite jet where the source is $\mathrm{s}(\mu) := (\mu(x_1), \ldots, \mu(x_p)) \in \mathbb{C}^p$ and the target is $\mathrm{t}(\mu) := (\mu(u_1), \ldots, \mu(u_n)) \in \mathbb{C}^n$. Thus, a Taylor series is a $\mathbb{C}$-point of an algebraic quasi–affine variety. Its Zarisky cloture is an affine variety defined by the ideal $\mathfrak{c}$. The dimension of the solutions space of (13) is the number of arbitrary constants appearing in the Taylor series solutions μ when the

source point $\mathrm{x} := \mathrm{s}(\mu) \in \mathbb{C}^p$ is determined. Let K be the fractions field $\mathrm{Frac}(R/\mathfrak{c})$. Recall that the *transcendence degree* of a field extension K/k is the greatest number of elements in K which are k-algebraically independent. The degree $[K : \mathrm{k}]$ is the dimension of K as a k-vector space. When $\mathrm{tr\ deg}(K/\mathrm{k}) = 0$, the field K is algebraic over k and $[K : \mathrm{k}] < \infty$. If $f \in C$, we denote $\mathrm{rank}(f) := (v, d)$ where $v := \mathrm{ld}\, f$ and $d := \deg(f, v)$. Let

$$\begin{aligned} \mathrm{rank}\, C &:= \{\mathrm{rank}(f) \mid f \in C\} \\ \mathrm{ld}\, C &:= \{\mathrm{ld}(f) \mid f \in C\} \\ \dim C &:= \mathrm{card}\,(\Theta U \setminus \Theta(\mathrm{ld}\, C)) \\ \deg C &:= \prod_{f \in C} \deg(f, \mathrm{ld}\, f). \end{aligned}$$

PROPOSITION 2. $\dim C = \mathrm{tr\ deg}(K/\mathrm{k})$ *is the dimension of the solutions space of (13). If* $\dim C = 0$ *then the cardinal of the solutions space is finite and equal to* $\deg C = [K : \mathrm{k}]$.

3.3 Differential elimination

Let $U = U_1 \sqcup U_2$ be a partition of the alphabet U. A ranking which eliminates the indeterminates of U_2 is such that

$$\forall v_1 \in \Theta U_1, \forall v_2 \in \Theta U_2, \quad v_2 \succ v_1. \tag{14}$$

Assume that C is a characteristic set of the prime differential ideal $\mathfrak{c} = \sqrt{[C]} : H_C^\infty$ w.r.t. the elimination ranking $\Theta U_2 \succ \Theta U_1$. Let $R_1 := k\{U_1\}$ be the differential polynomials k-algebra generated by the set U_1. Consider the set $C_1 := C \cap R_1$ and the differential ideal $\mathfrak{c}_1 := \mathfrak{c} \cap R_1$.

PROPOSITION 3. C_1 *is a characteristic set of* $\mathfrak{c}_1$.

Consider the differential field of fractions $K := \mathrm{Frac}(R/\mathfrak{c})$ and denote by $\alpha : R \to K$ the canonical k-algebra morphism. Let K_1 be the differential subfield of K generated by the set $\alpha(R_1)$. Then K_1 is the fraction field associated to the prime differential ideal $\mathfrak{c}_1 := \mathfrak{c} \cap R_1$. The partition of the characteristic set

$$C = C_1 \sqcup C_2 \quad (\text{i.e. } C_2 := C \setminus C_1). \tag{15}$$

enables us to study the field extension K/K_1.

PROPOSITION 4. $\mathrm{tr\ deg}(K/K_1) = \dim C_2$. *If* $\dim C_2 = 0$ *then* $[K : K_1] = \deg C_2$.

3.4 The system (7) revisited

3.4.1 Prolongation algorithm

Our aim, here, is to prolong the action of $\Phi \subset \mathrm{J}_*^\infty(\mathbb{C}^2, \mathbb{C}^2)$ on the manifold $M := \mathrm{J}^n(\mathbb{C}, \mathbb{C})$. For each integer $q \geq 0$, define

$$\begin{aligned} \mathrm{k}^{(q)} &:= \mathbb{Q}(x,\, y,\, y_1, \ldots,\, y_q) \\ R^{(q)} &:= \mathrm{k}^{(q)}\{\bar{x},\, \bar{y},\, \bar{y}_1, \ldots,\, \bar{y}_q\} \end{aligned}$$

The differential field $\mathrm{k}^{(q)}$ is the coefficients field of the ring of differential polynomials $R^{(q)}$ endowed with the set of derivations $\left\{\frac{\partial}{\partial x},\, \frac{\partial}{\partial y},\, \ldots,\, \frac{\partial}{\partial y_q}\right\}$. Let us assume that the Lie defining equations of Φ are given by a characteristic set $C^{(0)} \subset R^{(0)}$. The $\mathcal{D}$-groupoid $\Phi^{(q)}$ acting on J^q and prolonging the action of Φ is characterized by a characteristic set $C^{(q)} \subset R^{(q)}$. The prolongation formulae [15] of the point transformation $(x, y) \to (\xi(x, y),\, \eta(x, y))$ are of the form

$$\bar{y}_q = \eta_q(x,\, y, \ldots,\, y_q),$$

where $\bar{y} = \eta(x,\, y)$ if $q = 0$. The computation of the characteristic set $C^{(q)}$ is done incrementally using the infinite Cartan field $D_x := \frac{\partial}{\partial x} + y_1 \frac{\partial}{\partial y} + y_2 \frac{\partial}{\partial y_1} + \cdots$

$$\begin{aligned} \eta_q &:= D_x \eta_{q-1} \cdot (D_x \xi)^{-1} \\ C^{(q)} &:= C^{(q-1)} \cup \left\{\bar{y}_q - \mathsf{normal\_form}\left(\eta_q,\, C^{(q-1)}\right)\right\} \end{aligned}$$

PROPOSITION 5. *If* $C^{(0)}$ *is a* quasi-linear *characteristic set of* Φ *then* $C^{(q)}$ *is a* quasi-linear *characteristic set of* $\Phi^{(q)}$ *w.r.t. the elimination ranking* $\Theta \bar{y}_q \succ \Theta \bar{y}_{q-1} \succ \cdots \succ \Theta\{\bar{y}, \bar{x}\}$.

The previous proposition gives an efficient method to prolong a $\mathcal{D}$-groupoid Φ without the explicit knowledge of transformations.

3.4.2 EPB with fixed target

Let us compute a characteristic set $C[\bar{f}] \subset R^{(n)}\{f\}$ for the PDE system (7) where $\bar{f}$ is fixed $\mathbb{Q}$-rational function. First, prolong $C^{(0)}$ up to the order $n+1$ as above. Then $C[\bar{f}]$ is obtained by substituting in $C^{(n+1)}$ the indeterminate y_{n+1} by the symbol f and the indeterminate $\bar{y}_{n+1}$ by the rational function $\bar{f}(\bar{x}, \cdots, \bar{y}_n)$.

EXAMPLE 4. *For the EPB* $(\mathrm{J}^1(\mathbb{C}, \mathbb{C}), \Phi_3)$, *we have*

$$\begin{gathered} \bar{p} - \bar{y}_x - p \bar{y}_y = 0, \\ \bar{y}_{xx} + 2p \bar{y}_{xy} + p^2 \bar{y}_{yy} + f\ \bar{y}_y - \bar{f}(\bar{x},\, \bar{y},\, \bar{p}) = 0, \\ \bar{x}_x - 1 = 0,\, \bar{x}_y = 0,\, \bar{x}_p = 0,\, \bar{y}_p = 0,\, \bar{y}_y \neq 0. \end{gathered} \tag{16}$$

These equations constitute a quasi-linear characteristic set w.r.t. the elimination ranking $\Theta f \succ \Theta \bar{p} \succ \Theta \bar{y} \succ \Theta \bar{x}$. *Hence, the associated differential ideal is prime.*

COROLLARY 1. *The PDE system (7) (where* $\bar{f}$ *is a fixed* $\mathbb{Q}$*-rational function) is a quasi–linear characteristic set* $C[\bar{f}] \subset R^{(n)}\{f\}$ *w.r.t the elimination ranking* $\Theta f \succ \Theta \bar{y}_n \succ \cdots \succ \Theta\{\bar{y}, \bar{x}\}$.

3.5 Brute-force method

Using ROSENFELD-GRÖBNER we compute a new characteristic set $C[\bar{f}]$ of the PDE system (7) w.r.t. the new ranking $\Theta\{\bar{y}_n, \cdots, \bar{y}_1, \bar{x}\} \succ \Theta\{f\}$. We make the partition of $C := C[\bar{f}]$ as in (15)

$$C = C_f \sqcup C_\varphi \tag{17}$$

where $C_f := C \cap \mathrm{k}^{(n)}\{f\}$ and $C_\varphi := C \setminus C_f$.

PROPOSITION 6. *The transformation* φ *does exist for* almost any *function* f *satisfying the PDE system associated to the characteristic set* $C_f[\bar{f}]$. *The function* $\bar{\mathrm{x}} = \varphi(x)$ *is solution of the PDE system associated to* $C_\varphi[\bar{f}]$.

If $\dim C_\varphi[\bar{f}] = 0$, one can calculate φ by an algebraic process without integrating differential equations.

DEFINITION 9. *When* $\dim C_\varphi[\bar{f}] = 0$, *the algebraic system associated to* $C_\varphi[\bar{f}]$ *is called the* necessary form of the change of coordinates $\bar{\mathrm{x}} = \varphi(\mathrm{x})$.

Example 5. *Consider the EPB* $(\mathrm{J}^1(\mathbb{C},\mathbb{C}),\Phi_3)$. *Suppose that the target* $\mathcal{E}_{\bar f}$ *is the Airy equation*

$$\bar y'' = \bar x \bar y.$$

In this case, Rosenfeld-Gröbner *returns* $C_\varphi[\bar f]$ *and* $C_f[\bar f]$ *resp. given by (18) and (19)*

$$\begin{array}{rcl} \bar y_{xx} &=& -f\bar y_y + pf_p\bar y_y - 1/2\,p^2 f_{pp}\bar y_y + \bar y f_y - 1/2\,\bar y f_{xp} \\ && -1/2\,\bar y f_{pp} f + 1/4\,\bar y {f_p}^2 - 1/2\,\bar y p f_{yp} \\ \bar y_{xy} &=& -1/2\,f_p\bar y_y + 1/2\,pf_{p,p}\bar y_y \\ \bar y_{yy} &=& -1/2\,f_{pp}\bar y_y, \quad \bar y_p = 0, \\ \bar x &=& f_y - 1/2\,f_{xp} - 1/2\,f_{pp}f + 1/4\,{f_p}^2 - 1/2\,pf_{yp} \end{array} \tag{18}$$

$$\begin{array}{rcl} f_{xxp} &=& 2\,f_{xy} + f_p f_{xp} - 2 + p^2 f_{yyp} - f_{pp}f_x + \cdots \\ f_{xyp} &=& 2\,f_{yy} - pf_{yyp} - f_{ypp}f - f_{pp}f_y + f_p f_{yp} \\ f_{xpp} &=& f_{yp} - pf_{ypp} \\ f_{ppp} &=& 0. \end{array} \tag{19}$$

We have $\dim C_\varphi[\bar f] = 3$ *which means that the transformation* $\bar{\mathrm{x}} = \varphi(\mathrm{x})$, *when* f *satisfies* $C_f[\bar f]$, *depends on 3 arbitrary constants.*

Example 6. *Consider the EPB* $(\mathrm{J}^1(\mathbb{C},\mathbb{C}),\Phi_1)$ *where* Φ_1 *is defined in table 1. Assume that the target equation* $\mathcal{E}_{\bar f}$ *is*

$$\bar y'' = \bar y^3.$$

Here, Rosenfeld-Gröbner *returns* $C_\varphi[\bar f]$ *and* $C_f[\bar f]$ *resp. given by (20) and (21)*

$$\begin{array}{rcl} \bar y^2 &=& 1/12\,(4\,f_y - 2\,f_{xp} - 2\,f_{pp}f - 2\,pf_{yp} + {f_p}^2), \\ \bar x &=& x, \end{array} \tag{20}$$

$$\begin{array}{rcl} f_{xxxp} &=& (4\,f_y - 2\,f_{xp} - 2\,f_{pp}f - 2\,pf_{yp} + {f_p}^2)^{-1}\times \\ && \vdots \\ f_{xxyp} &=& (4\,f_y - 2\,f_{xp} - 2\,f_{pp}f - 2\,pf_{yp} + {f_p}^2)^{-1}\times \\ && \vdots \\ f_{xyyp} &=& (4\,f_y - 2\,f_{xp} - 2\,f_{pp}f - 2\,pf_{yp} + {f_p}^2)^{-1}\times \\ && \vdots \\ f_{xpp} &=& f_{yp} - pf_{ypp} \\ f_{ppp} &=& 0. \end{array} \tag{21}$$

Consequently $\dim C_\varphi[\bar f] = 0$ *and* $\deg C_\varphi[\bar f] = 2$. *Thus,* φ *is the algebraic transformation of degree 2, given by equations (20).*

3.6 Discrete symmetries $\mathcal{D}$-groupoids

The self–equivalence problem, is in fact, the EPB when the PDE system (7) is *specialized* by substituting the symbol f by the value $\bar f(\mathrm{x})$, that is

$$f := \bar f(x, y, \ldots, y_n). \tag{22}$$

After specialization, the differential system $C_f[\bar f]$ constraining the function f is automatically satisfied (since there exists at least one solution $\bar{\mathrm{x}} = \sigma(\mathrm{x})$ of the problem, namely $\sigma = \mathrm{Id}$). The symmetries σ are solutions of a characteristic set $C_\sigma[\bar f]$ obtained form $C_\varphi[\bar f]$ by the specialization (22).

By definition, the degree of an algebraic transformation $\bar{\mathrm{x}} = \varphi(x)$ is the generic number of points $\bar{\mathrm{x}}$ when x is determined.

Theorem 1. *The following conditions are equivalent*

(1) $\dim(C_\varphi[\bar f]) = 0$,
(2) $\dim(\mathcal{S}_{\bar f}) = 0$,
(3) $\deg(\mathcal{S}_{\bar f}) < \infty$.

In this case, $\deg \mathcal{S}_{\bar f} = \deg(C_\varphi[\bar f]) = \deg\varphi$.

Proof. Define

$$\mathcal{G}_{\bar f} := \left\{ (\jmath_{\mathrm{x}} f,\, \jmath_{\mathrm{x}}\varphi,\, \jmath_{\bar{\mathrm{x}}}\bar f) \in \mathcal{G} \mid \bar f \text{ determined} \right\}.$$

$\mathcal{G}_{\bar f}$ is an algebraic covering of M defined by the characteristic set $C_\varphi[\bar f]$. The $\mathcal{D}$-groupoid $\mathcal{S}_{\bar f} \subset \mathcal{G}_{\bar f}$ is defined by differential system (8) i.e. the characteristic set $C_\sigma[\bar f]$. Figure 2 shows that $\mathcal{S}_{\bar f}$ acts simply transitively on $\mathcal{G}_{\bar f}$.

$$\begin{tikzcd} \jmath_{\mathrm{x}} f \arrow[r, "\varphi_0"] \arrow[dr, "\varphi"'] & \jmath_{\bar{\mathrm{x}}_0}\bar f \arrow[d, "\sigma"] \\ & \jmath_{\bar{\mathrm{x}}}\bar f \end{tikzcd}$$

Figure 2: *Simply transitive action of* $\mathcal{S}_{\bar f}$ *on* $\mathcal{G}_{\bar f}$ *where* $\bar{\mathrm{x}}_0 = \varphi_0(\mathrm{x})$ *and* $\bar{\mathrm{x}} = \varphi(\mathrm{x})$

Choose a point $\bar{\mathrm{x}}_0$ in M. For every $\varphi_0 \in \Gamma\Phi$, define the rational transformation $\mathcal{S}_{\bar f} \to \mathcal{G}_{\bar f}$

$$\jmath_{\bar{\mathrm{x}}_0}\sigma \to (\jmath_{\bar{\mathrm{x}}_0}\sigma) \circ (\jmath_{\mathrm{x}}\varphi_0), \quad (\sigma \in \Gamma\mathcal{S}_{\bar f}).$$

In fact, according to the Taylor series composition formulae, this transformation is birational. Thus, the one-to-one correspondence between the two algebraic varieties $\mathcal{G}_{\bar f}$ and $\mathcal{S}_{\bar f}$ is birational. Consequently, the two characteristic sets $C_\varphi[\bar f]$ and $C_\sigma[\bar f]$ have the same dimension and the same degree. $\square$

Lemma 1. *The rank of the characteristic set* $C_\varphi[\bar f]$ *is stable under the specialization (22) i.e.* $\operatorname{rank} C_\varphi[\bar f] = \operatorname{rank} C_\sigma[\bar f]$.

Proof. The specialization (22) transforms the characteristic set $C_\varphi[\bar f]$ to $C_\sigma[\bar f]$. A fall of the rank of $C_\varphi[\bar f]$ during the specialization contradicts the existence of birational correspondence between $\mathcal{G}_{\bar f}$ and $\mathcal{S}_{\bar f}$. $\square$

Remark 1. *When the transformation* $\bar{\mathrm{x}} := \varphi(\mathrm{x})$ *is locally bijective but not globally,* $\mathcal{S}_f$ *and* $\mathcal{S}_{\bar f}$ *need not to have the same degree. Indeed, consider again the groupoid* Φ_3 *and the equations*

$$y'' = \frac{6y^4 + x - 2{y'}^2}{2y} \text{ and } \bar y'' = 6\bar y^2 + \bar x$$

which are equivalent under $(\bar x = x,\ \bar y = y^2)$. *The corresponding symmetry group are respectively given by*

$$\Gamma\mathcal{S}_f = \{(x,y) \to (x, \lambda y) \mid \lambda^2 = 1\} \text{ and } \Gamma\mathcal{S}_{\bar f} = \{\mathrm{Id}\}.$$

They have the same dimension but different cardinal.

3.7 Expression swell

In practice, the above brute–force method, which consists of applying Rosenfeld-Gröbner to the PDE system (7), is rarely effective due to expressions swell. Much of the examples treated here and in [6], using our algorithm ChgtCoords, can not be treated with this approach.

It seems that the problem lies in the fact that we can not separate the computation of $C_\varphi[\bar f]$ from that of $C_f[\bar f]$ which contains, very often, big expressions.

An other disadvantage of the above method is that we have to restart computation from the very beginning if the target equation is changed. In the next section, we propose our algorithm ChgtCoords to compute the transformation φ alone and in terms of differential invariants. These invariants are provided by Cartan method for a generic f which means that we have not re-apply Cartan method if the target equation is changed and a big part of calculations is generic. Furthermore, the computation of φ in terms of differential invariants reduces significantly the size of the expressions.

4. USING CARTAN'S METHOD

In this paper, differential invariants are obtained using Cartan's equivalence method. We refer the reader to [3, 13, 16, 7] for an expanded tutorial presentation and application to second order ODE. When applied Cartan's method furnishes a finite set of fundamental invariants and a certain number of invariant derivations generating the differential field of invariant functions.

EXAMPLE 7. *Consider the EPB* $(J^1(\mathbb{C},\mathbb{C}),\Phi_3)$. *The PDE system (7) reads*

$$\underbrace{\begin{pmatrix}\mathrm{d}\bar p-\bar f(\bar x,\bar y,\bar p)\mathrm{d}\bar x\\ \mathrm{d}\bar y-\bar p\mathrm{d}\bar x\\ \mathrm{d}\bar x\end{pmatrix}}_{\omega_{\bar f}}=\underbrace{\begin{pmatrix}a_1&a_2&0\\0&a_3&0\\0&0&1\end{pmatrix}}_{S(\mathrm{a})}\underbrace{\begin{pmatrix}\mathrm{d}p-f(x,y,p)\mathrm{d}x\\ \mathrm{d}y-p\mathrm{d}x\\ \mathrm{d}x\end{pmatrix}}_{\omega_f}$$

with $\det(S(\mathrm{a}))\neq 0$. *In accordance with Cartan, this system is lifted to the linear Pfaffian system*

$$S(\bar{\mathrm{a}})\ \omega_{\bar f}=S(\mathrm{a})\ \omega_f$$

defined on the manifold of local coordinates $(\mathrm{x},\mathrm{a},\bar{\mathrm{x}},\bar{\mathrm{a}})$. *After two normalizations and one prolongation, Cartan's method yields three fundamental invariants* ($p=y'$ *and* $a=a_3$)

$$\begin{aligned}&I_1=-\frac{1}{4}(f_p)^2-f_y+\frac{1}{2}D_xf_p,\quad I_2=\frac{f_{ppp}}{2a^2},\\&I_3=\frac{f_{yp}-D_xf_{pp}}{2a},\end{aligned}\tag{23}$$

and the invariant derivations

$$\begin{aligned}&X_1=\frac{1}{a}\frac{\partial}{\partial p},\quad X_3=D_x-\frac{1}{2}f_pa\frac{\partial}{\partial a},\quad X_4=a\frac{\partial}{\partial a},\\&X_2=\frac{1}{a}\frac{\partial}{\partial y}+\frac{1}{2}\frac{f_p}{a}\frac{\partial}{\partial p}-\frac{1}{2}f_{pp}\frac{\partial}{\partial a},\end{aligned}\tag{24}$$

where $D_x=\frac{\partial}{\partial x}+p\frac{\partial}{\partial y}+f(x,y,p)\frac{\partial}{\partial p}$.

When $\dim(\mathcal{S}_f)=0$, *the additional parameter* a *can be (post)normalized by fixing some invariant to some suitable value. In this manner one constructs invariants defined on* M *(not depending on the additional parameter).*

THEOREM 2 (OLVER [16]). *If* $\dim(\mathcal{S}_{\bar f})=0$, *then there exist exactly* m *functionally independent specialized invariants* $I_1[\bar f],\cdots,I_m[\bar f]$.

Note that the invariants $I_1[\bar f],\cdots,I_m[\bar f]$ are functionally independent if and only if $\mathrm{d}I_1[\bar f]\wedge\cdots\wedge\mathrm{d}I_m[\bar f]\neq 0$. Note also that if the function $\bar f$ is rational, then the specialized invariants $I[\bar f]:M\to\mathbb{C}$ are algebraic functions. In the sequel, we use the notation $I_{i;j\cdots k}$ to denote the differential invariant $X_k\cdots X_j(I_i)$.

4.1 Computation of φ

Suppose that the $\mathcal{D}$-groupoid $\mathcal{S}_{\bar f}$ is zerodimensional. Then, according to the theorem 2, there exists m functionally independent invariants $F_k:=I_k[\bar f]$, $1\leq k\leq m$. This implies that the algebraic (non differential) system

$$\{F_1(\bar{\mathrm{x}})=I_1,\ldots,F_m(\bar{\mathrm{x}})=I_m\}\tag{25}$$

is locally invertible and has a finite number of solutions

$$\bar{\mathrm{x}}=F^{-1}(I_1,\ldots,I_m).\tag{26}$$

The specialization of $I_1,\ldots,I_m$ on the source function f yields

$$\bar{\mathrm{x}}=F^{-1}(I_1[f],\ \ldots,I_m[f]).\tag{27}$$

Let C denote the (non differential) characteristic set associated to the system (25) w.r.t. the elimination ranking $\{\bar x,\bar y,\ldots,\bar y_n\}\succ\{I_1,\ldots,I_m\}$. Thus, C describes the inversion (26). The most simple situation happens when $\deg(C)=1$. In this case, the necessary form of the change of coordinates φ is the rational transformation defined by C.

EXAMPLE 8. *Consider the EPB* $(\mathrm{J}^1(\mathbb{C},\mathbb{C}),\Phi_3)$ *and the target equation* $\mathcal{E}_{\bar f}$ *introduced by G. Reid [17]*

$$\bar y''=\frac{\bar y'}{\bar x}+\frac{4\bar y^2}{\bar x^3}.$$

The following invariants are functionally independent

$$\begin{aligned}\bar I_{1;23}=-20\frac{1}{\bar a\bar x^4},\ \bar I_{1;31}=8\frac{1}{\bar a\bar x^3},\ \bar I_1=\frac{3}{4\bar x^2}+8\,\frac{\bar y}{\bar x^3},\\ \bar I_{1;3}=\frac{-3\,\bar x-48\,\bar y+16\,\bar p\bar x}{2\bar x^4}.\end{aligned}$$

We normalize the parameter $\bar a$ *by setting* $\bar I_{1,23}=-20$. *The characteristic set* C *is*

$$\begin{cases}\bar p=-\dfrac{3}{32}+\dfrac{3}{512}{I_{1;31}}^2I_1+\dfrac{1}{4096}I_{1;3}{I_{1;31}}^3,\\[2ex] \bar y=-\dfrac{3}{256}I_{1;31}+\dfrac{1}{4096}I^3_{I_{1;31}},\\[2ex] \bar x=\dfrac{1}{8}I_{1;31},\end{cases}$$

which gives the sought necessary form of φ. *As a byproduct we deduce that the symmetry group* $\Gamma\mathcal{S}_{\bar f}=\{\mathrm{Id}\}$.

Let us return to the general situation, that is when $\deg(C)$ is strictly bigger than 1. We have two cases. First, $\deg(C)=\deg(\mathcal{S}_{\bar f})$ and then φ is the algebraic transformation defined by C. Second, $\deg(C)>\deg(\mathcal{S}_{\bar f})$. In this case, to obtain the transformation φ, we have to look for m other functionally independent invariants such that the new characteristic set C has degree equal to $\deg(\mathcal{S}_{\bar f})$.

EXAMPLE 9. *Consider the EPB* $(\mathrm{J}^1(\mathbb{C},\mathbb{C}),\Phi_3)$ *and the target equation* $\mathcal{E}_{\bar f}$ *(number 8 in [9])*

$$\bar y''=\bar y^3+\bar x\bar y$$

which the corresponding symmetry group is

$$\Gamma\mathcal{S}_{\bar f}=\left\{(x,y)\to(x,\ \lambda y)\,|\lambda^2=1\right\}.$$

One can verify that I_1, $I_{1;13}$ *and* $I_{1;133}$, *when specialized on the considered equation, are functionally independent. In*

this case, the associated characteristic set C is

$$\left\{\begin{array}{lcl} \bar{p} & = & -\dfrac{\left(4\bar{x}^2+2I_1\bar{x}-3I_{1;33}-2{I_1}^2\right)\bar{y}}{3(I_{1;3}+1)}, \\ \bar{y}^2 & = & -\dfrac{1}{3}\bar{x}-\dfrac{1}{3}I_1, \\ \bar{x}^3 & = & -\dfrac{3}{2}I_1\bar{x}^2+\dfrac{3}{4}I_{1;33}\bar{x}-\dfrac{3}{4}I_{1;3}-\dfrac{3}{8}{I_{1;3}}^2+\dfrac{3}{4}I_{1;33}I_1 \\ & & +\dfrac{1}{2}{I_1}^3-\dfrac{3}{8}. \end{array}\right.$$

The degree of this set is equal to 6 which is different from the degree of the symmetry groupoid.

However, if instead of the above invariants we consider the invariants $K_1 := I_{1;233}/I_{1;31}$, $K_2 := I_{1;234}/I_{1;31}$ and $K_3 := I_{1:231}/I_{1;31}^2$, we obtain

$$\left\{\begin{array}{lcl} \bar{p} & = & -K_1\bar{y}, \\ \bar{y}^2 & = & \dfrac{1}{6}K_3, \\ \bar{x} & = & -\dfrac{1}{6}K_3+K_1. \end{array}\right.$$

This characteristic gives the necessary form of φ since it has degree two.

4.1.1 Heuristic of degree reduction

In practice, one has to search the invariants giving the required degree in the algebra of invariants. However, this is not an easy task since this algebra can be very large (although it is algorithmic). For this reason we provide an important heuristic which enables us to obtain the desired invariants. This heuristic is explained in the following example.

Example 10. *Consider the Emden Fowler equation (9) and the $\mathcal{D}$-groupoid of transformations Φ_3. We have already computed the corresponding symmetry groupoid. The specialization of the invariants I_1, $I_{1;13}$ and $I_{1;133}$ gives three functionally independent functions. As explained above, we obtain the following characteristic set computed w.r.t. the ranking $\bar{p} \succ \bar{y} \succ \bar{x} \succ I_1 \succ I_{1;3} \succ I_{1;33}$*

$$\left\{\begin{array}{lcl} \bar{p} & = & \left(\dfrac{3}{8}I_1-\dfrac{1}{4}\dfrac{I_{1;33}}{I_1}+\dfrac{1}{3}\dfrac{{I_{1;3}}^2}{{I_1}^2}\right)\bar{x}\bar{y}-\dfrac{1}{6}\dfrac{I_{1;3}}{I_1}\bar{y}, \\ \bar{y}^3 & = & \left(-\dfrac{9}{4}-2\dfrac{{I_{13}}^2}{{I_1}^3}+\dfrac{3}{2}\dfrac{I_{1;33}}{{I_1}^2}\right)\bar{x}-\dfrac{I_{1;3}}{{I_1}^2}, \\ \bar{x}^2 & = & 4\left(\dfrac{I_{1;3}I_1}{9{I_1}^3-8{I_{1;3}}^2+6I_{1;33}I_1}\right)\bar{x} \\ & & +8\dfrac{{I_1}^2}{9{I_1}^3-8{I_{1;3}}^2+6I_{1;33}I_1}. \end{array}\right. \quad (28)$$

Comparing with the $\mathcal{D}$-groupoid of symmetries (10) we deduce that, in contrary to $\bar{y}$, the degree of $\bar{x}$ must be reduced to one. This can be done in the following manner. First, observe that the Lie defining equations of Φ_3, more exactly $\bar{x}_p = 0$, implies that $X_1(\bar{x}) = 0$ where $X_1 = \frac{\partial}{a\partial p}$ is the invariant derivation (24). Now, differentiate the last equation of the characteristic set, which we write as $\bar{x}^2 = A\bar{x} + B$, w.r.t the derivation X_1. We find $A_{;1}\bar{x} + B_{;1} = 0$. The coefficient of $\bar{x}$ in this equation, which is invariant, could not vanish (since it is not identically zero when specializing on the Emden–Fowler equation). Thus, $\bar{x} = -\dfrac{B_{;1}}{A_{;1}}$ or explicitly

$$\bar{x} = -2\frac{KI_{1;1}+I_1K_{;1}}{KI_{1;31}+I_{1;3}K_{;1}} \quad \textit{with } K = \frac{I_1}{9{I_1}^3-8{I_{1;3}}^2+6I_{1;33}I_1}. \quad (29)$$

The necessary form of the change of coordinates φ is then given by (29) and the two first equations of (28).

The above reasoning can be summarized as follows

Procedure ChgtCoords
Input : $\mathcal{E}_{\bar{f}}$ and Φ such that $\dim(\mathcal{S}_{\bar{f}}) = 0$
Output : $\bar{\mathrm{x}} = \varphi(\mathrm{x})$ the necessary form of the change of coordinates
1- Find m functionally independent invariants $(I_1[\bar{f}], \ldots, I_m[\bar{f}])$ defined on M.
2- Compute a char. set C of the algebraic system (26).
3- If $\deg(C) = 1$ then Return C.
4- Compute $\mathcal{S}_{\bar{f}}$ with Rosenfeld-Gröbner.
5- WHILE $\deg(C) \neq \deg(\mathcal{S}_{\bar{f}})$ DO
  Reduce the degree of C.
END DO
6- Return C.

5. THE SOLVER

5.1 Precalculation of φ

5.1.1 The first step : the adapted $\mathcal{D}$-groupoid

Let $\Phi_1, \ldots, \Phi_7 \subset \mathrm{J}^{\infty}_{*}(\mathbb{C}^2, \mathbb{C}^2)$ denote the $\mathcal{D}$-groupoids defined in the table 1 above. It is not difficult to see that $\Phi_1 \subset \Phi_3 \subset \Phi_5$ and $\Phi_2 \subset \Phi_4 \subset \Phi_6$ and finally $\Phi_5, \Phi_6 \subset \Phi_7$.

Let $\mathrm{d}(\mathcal{E}_f, \Phi) := \dim(\mathrm{aut}(\mathcal{E}_f) \cap \Phi)$ where $\mathrm{aut}(\mathcal{E}_f)$ is the contact symmetry $\mathcal{D}$-groupoid of the second order ODE $\mathcal{E}_f$. Let $\mathrm{d}_i := \mathrm{d}(\mathcal{E}_f, \Phi_i)$ for $1 \le i \le 7$.

Definition 10 (Signature). *The* signature *of $\mathcal{E}_f$ is*

$$\mathrm{sign}(\mathcal{E}_f) := ((\mathrm{d}_1, \mathrm{d}_3, \mathrm{d}_5), (\mathrm{d}_2, \mathrm{d}_4, \mathrm{d}_6), \mathrm{d}_7).$$

Clearly, $(\mathrm{d}_1 \le \mathrm{d}_3 \le \mathrm{d}_5 \le \mathrm{d}_7)$ and $(\mathrm{d}_2 \le \mathrm{d}_4 \le \mathrm{d}_6 \le \mathrm{d}_7)$. Recall that the calculation of theses dimensions does not require solving differential equations. We shall say that the signature $\mathrm{sign}(\mathcal{E}_f)$ *matches* the signature $\mathrm{sign}(\mathcal{E}_{\bar{f}})$ if and only if $\mathrm{d}_7 = \bar{\mathrm{d}}_7$ and ($s_1 = \bar{s}_1$ or $s_2 = \bar{s}_2$) where s_1 and s_2 stand for $(\mathrm{d}_1, \mathrm{d}_3, \mathrm{d}_5)$ and $(\mathrm{d}_2, \mathrm{d}_4, \mathrm{d}_6)$ resp. Two second order ODE $\mathcal{E}_f$ and $\mathcal{E}_{\bar{f}}$ are said to be *strongly equivalent* if

$$\exists \Phi \in \{\Phi_1, \cdots, \Phi_7\}, \exists \varphi \in \Phi,\ \varphi_* \mathcal{E}_f = \mathcal{E}_{\bar{f}},\ \mathrm{d}(\mathcal{E}_{\bar{f}}, \Phi) = 0.$$

Lemma 2. *If $\mathcal{E}_f$ and $\mathcal{E}_{\bar{f}}$ are strongly equivalent then their signatures match.*

Definition 11 (Adapted $\mathcal{D}$-groupoid). *A $\mathcal{D}$-groupoid Φ is said to be* adapted *to the ODE $\mathcal{E}_f$ if $\mathrm{d}(\mathcal{E}_f, \Phi) = 0$ and Φ is maximal among $\Phi_1, \cdots, \Phi_7$ satisfying this property.*

	Transformations	Equation number according to Kamke's book
Φ_1	$\bar{x} = x,\ \bar{y} = \eta(x, y)$,	1, 2, 4, 7, 10, 21, 23, 24, 30, 31, 32, 40, 42, 43, 45, 47, 50
Φ_3	$\bar{x} = x + C,\ \bar{y} = \eta(x, y)$,	11, 78, 79, 87, 90, 91, 92, 94, 97, 98, 105, 106, 156, 172
Φ_5	$\bar{x} = \xi(x),\ \bar{y} = \eta(x, y)$,	Null
Φ_2	$\bar{x} = \xi(x, y),\ \bar{y} = y$,	81, 89, 133, 134, 135, 237
Φ_4	$\bar{x} = \xi(x, y),\ \bar{y} = y + C$,	11, 79, 87, 90, 92, 93, 94, 97, 98, 99, 105, 106, 172, 178
Φ_6	$\bar{x} = \xi(x, y),\ \bar{y} = \eta(y)$,	80, 86, 156, 219, 233
Φ_7	$\bar{x} = \xi(x, y),\ \bar{y} = \eta(x, y)$,	3, 5, 6, 8, 9, 27, 44, 52, 85, 95, 108, 142, 144, 145, 147, 171, 211, 212, 238

Table 1.

The above table associates to each equation in the third column its adapted groupoids. For instance, the first Painlevé equation (number 3) appears in the last row which means that its adapted $\mathcal{D}$-groupoid is the point transformations $\mathcal{D}$-groupoid Φ_7 . To the Emden–Fowler equation, number 11, we associate the $\mathcal{D}$-groupoids Φ_3 and Φ_4. In the case of homogeneous linear second order ODE (e.g. Airy equation, Bessel equation, Gauß hyper-geometric equation) we prove that, generically, the adapted $\mathcal{D}$-groupoid is Φ_4.

5.1.2 The second step

Once the list of adapted $\mathcal{D}$-groupoids Φ is known, we proceed by computing the necessary form of the change of coordinates $\varphi \in \Phi$ using ChgtCoords. Doing so, we construct a MAPLE table indexed by Kamke's book equations and where entries corresponding to the index $\mathcal{E}_{\bar{f}}$ are:

1- the signature of $\mathcal{E}_{\bar{f}}$,
2- the list of the adapted $\mathcal{D}$-groupoids Φ of $\mathcal{E}_{\bar{f}}$,
3- the necessary form of the change of coordinates $\varphi \in \Phi$.

For instance, the entries associated to Rayleigh equation $y'' + {y'}^4 + y = 0$ are:

1- the signature $((0,1,1),(1,1,1),1)$,
2- the $\mathcal{D}$-groupoid Φ_1,
3- the necessary form of the change of coordinates

$$\left\{\begin{array}{lcl} \bar{p} & = & -36\dfrac{I_{2;1}}{72+72I_1+{I_{2;1}}^2}\bar{y}, \\ \bar{x} & = & x, \\ \bar{y}^3 & = & \dfrac{-1}{559872 I_{2;1}^2}(I_{2;1}^6 + 216 I_1 I_{2;1}^4 + 216 I_{2;1}^4 + 373248 \\ & & +15552 I_{2;1}^2 + 1119744 I_1^2 + 31104 I_1 I_{2;1}^2 \\ & & +1119744 I_1 + 373248 I_1^3 + 15552 I_1^2 I_{2;1}^2) \end{array}\right. \tag{30}$$

with the normalization $I_2/I_{2;1} = 1$. Invariants here are those generated by (23) and (24) plus the essential invariant $\bar{x} = x$.

5.2 Algorithmic scheme of the solver

To integrate a differential equation $\mathcal{E}_f$ our solver proceeds as follows

PROCEDURE Newdsolve
Input : $\mathcal{E}_f$
Output : An equation $\mathcal{E}_{\bar{f}}$ in Kamke's book and the transformation φ such that $\varphi_*(\mathcal{E}_f) = \mathcal{E}_{\bar{f}}$
1- Compute the signature of $\mathcal{E}_f$.
2- Select from the table the list of equations $\mathcal{E}_{\bar{f}}$ such that $\text{sign}(\mathcal{E}_{\bar{f}})$ matches $\text{sign}(\mathcal{E}_f)$.
3- FOR each equation $\mathcal{E}_{\bar{f}}$ in the selected list DO
 (i) Specialize, on $\mathcal{E}_f$, the necessary form of the change of coordinates associated to $\mathcal{E}_{\bar{f}}$. We obtain φ.
 (ii) If $\varphi \in \Phi$ and $\varphi_*(\mathcal{E}_f) = \mathcal{E}_{\bar{f}}$ then return $(\mathcal{E}_{\bar{f}}, \varphi)$.
END DO.

It is worth noticing that the time required to perform steps (i)- (ii) is very small. In fact, it is about one hundredth of a second using Pentium(4) with 256 Mo. The second feature of our solver is, contrarily to the symmetry methods, neither the table construction nor the algorithm of the solver involves integration of differential equations.

6. ACKNOWLEDGMENTS

We are thankful to Rudolf Bkouche and François Boulier for many useful discussions during the preparation of this article.

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